Succinic acid, 2-isopropoxyphenyl 2-(dimethylamino)ethyl ester

Inchi: InChI=1S/C17H25NO5/c1-13(2)22-14-7-5-6-8-15(14)23-17(20)10-9-16(19)21-12-11-18(3

InchiKey: SUAQZHACQTXAOI-UHFFFAOYSA-N

Formula: C17H25NO5

SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)OCCN(C)C

Mol. weight [g/mol]: 323.38

Physical Properties

Property code	Value	Unit	Source
gf	-269.46	kJ/mol	Joback Method
hf	-728.72	kJ/mol	Joback Method
hfus	39.70	kJ/mol	Joback Method
hvap	78.75	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	2.264		Crippen Method
mcvol	257.360	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2270.00		NIST Webbook
rinpol	2270.00		NIST Webbook
tb	807.02	K	Joback Method
tc	1008.70	K	Joback Method
tf	504.31	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.59	J/mol×K	807.02	Joback Method
cpg	789.81	J/mol×K	840.63	Joback Method
cpg	803.90	J/mol×K	874.25	Joback Method
cpg	816.89	J/mol×K	907.86	Joback Method
cpg	828.79	J/mol×K	941.47	Joback Method
cpg	839.60	J/mol×K	975.08	Joback Method
cpg	849.33	J/mol×K	1008.70	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357970&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume